

ABSTRACT

The present invention relates to crystallized molecules and molecular complexes which comprise the active site binding pocket or the FKBP12/FK506 binding pocket of calcineurin or close structural homologues to either binding pocket. This invention also relates to a data storage material encoded with the corresponding structure coordinates of those crystallized molecules or molecular complexes. Such data storage material is capable of displaying such molecules and molecular complexes as a graphical three-dimensional representation on a computer screen. In addition, this invention relates to methods of using the structure coordinates of those molecules or molecular complexes to solve the structure of homologous proteins. This invention also relates to methods of using the structure coordinates to screen and design compounds that bind to calcineurin or homologues thereof.

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